



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PUZ  
Title : Crystal Structure of a pre-translocation state MBP-Maltose transporter complex bound to AMP-PNP  
Authors : Oldham, M.L.; Chen, J.  
Deposited on : 2010-12-06  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

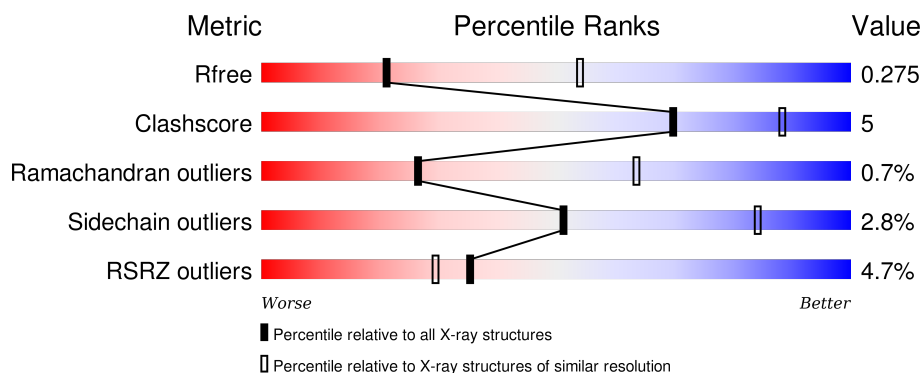
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	370	<div> <div>87%</div> <div>13%</div> </div>
2	F	514	<div>5%</div> <div>83%</div> <div>10%</div> <div>6%</div>
3	G	296	<div>3%</div> <div>81%</div> <div>11%</div> <div>5%</div>
4	A	381	<div>3%</div> <div>82%</div> <div>15%</div> <div>.</div>
4	B	381	<div>9%</div> <div>84%</div> <div>12%</div> <div>..</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PGV	F	4001	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 14697 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Maltose transporter subunit; periplasmic-binding component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	370	Total	C	N	O	S	0	0	0
			2880	1854	469	549	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	69	CYS	GLY	ENGINEERED MUTATION	UNP B1XC33
E	337	CYS	SER	ENGINEERED MUTATION	UNP B1XC33

- Molecule 2 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	481	Total	C	N	O	S	0	0	0
			3732	2452	594	669	17			

- Molecule 3 is a protein called Maltose transporter subunit; membrane component of ABC superfamily.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	282	Total	C	N	O	S	0	0	0
			2182	1461	348	364	9			

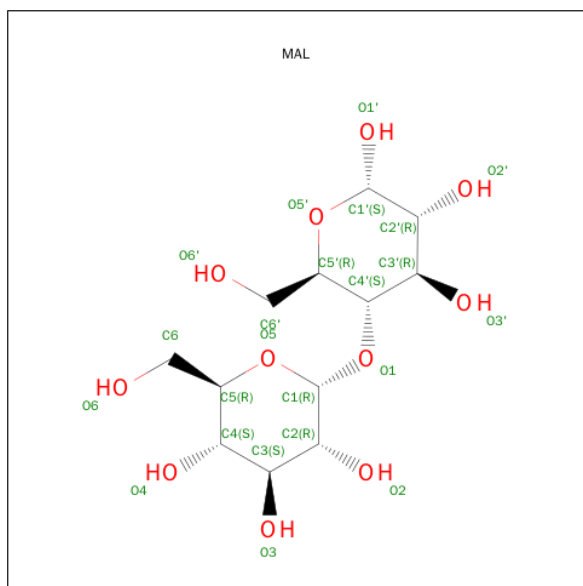
- Molecule 4 is a protein called Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			
4	B	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP B1XC34
A	373	SER	-	EXPRESSION TAG	UNP B1XC34
A	374	ALA	-	EXPRESSION TAG	UNP B1XC34
A	375	SER	-	EXPRESSION TAG	UNP B1XC34
A	376	HIS	-	EXPRESSION TAG	UNP B1XC34
A	377	HIS	-	EXPRESSION TAG	UNP B1XC34
A	378	HIS	-	EXPRESSION TAG	UNP B1XC34
A	379	HIS	-	EXPRESSION TAG	UNP B1XC34
A	380	HIS	-	EXPRESSION TAG	UNP B1XC34
A	381	HIS	-	EXPRESSION TAG	UNP B1XC34
B	372	ALA	-	EXPRESSION TAG	UNP B1XC34
B	373	SER	-	EXPRESSION TAG	UNP B1XC34
B	374	ALA	-	EXPRESSION TAG	UNP B1XC34
B	375	SER	-	EXPRESSION TAG	UNP B1XC34
B	376	HIS	-	EXPRESSION TAG	UNP B1XC34
B	377	HIS	-	EXPRESSION TAG	UNP B1XC34
B	378	HIS	-	EXPRESSION TAG	UNP B1XC34
B	379	HIS	-	EXPRESSION TAG	UNP B1XC34
B	380	HIS	-	EXPRESSION TAG	UNP B1XC34
B	381	HIS	-	EXPRESSION TAG	UNP B1XC34

- Molecule 5 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



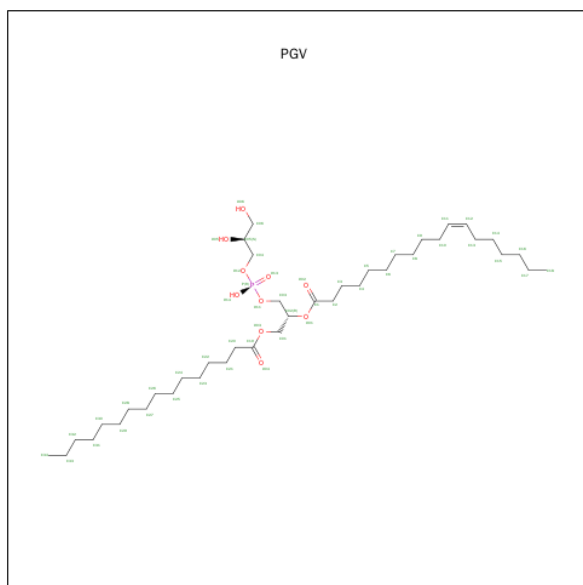
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			23	12	11		

- Molecule 6 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).

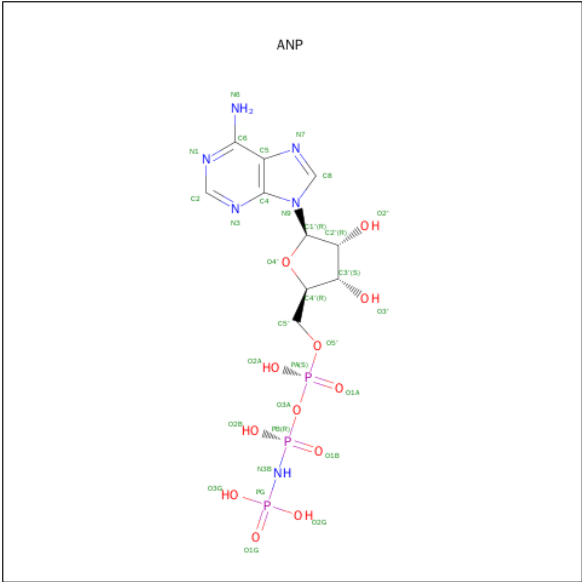


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
8	B	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

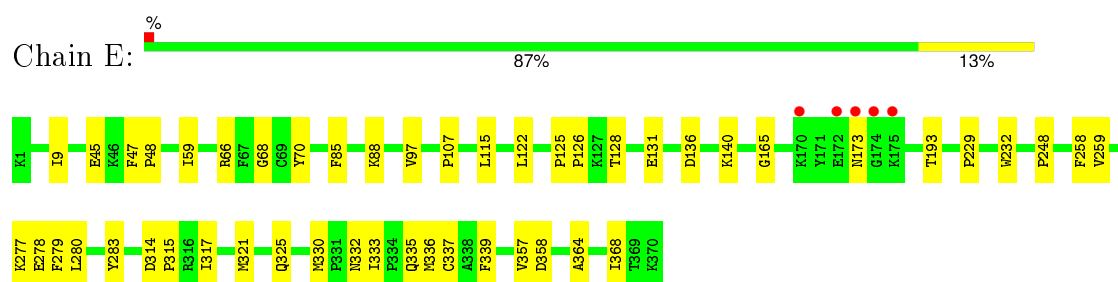
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	5	Total	O	0	0
			5	5		

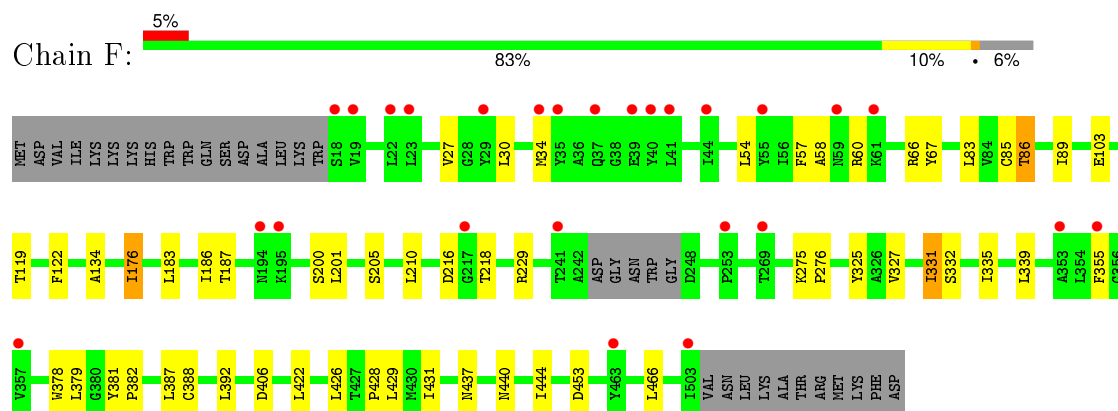
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

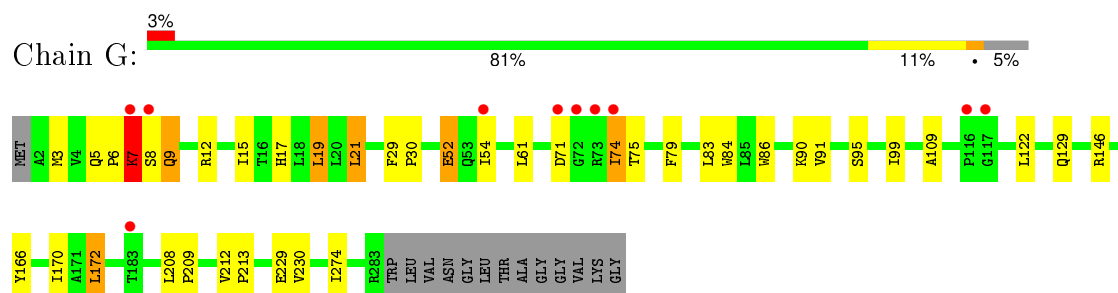
- Molecule 1: Maltose transporter subunit; periplasmic-binding component of ABC superfamily



- Molecule 2: Maltose transporter subunit; membrane component of ABC superfamily

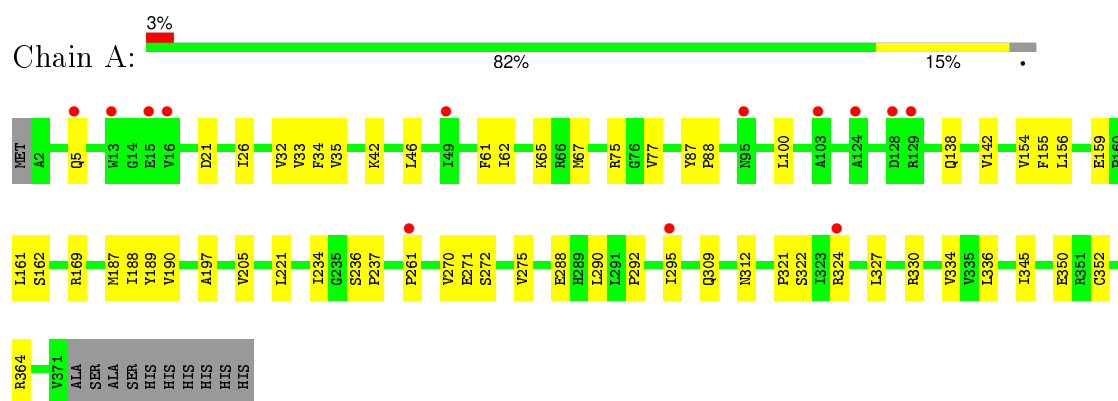


- Molecule 3: Maltose transporter subunit; membrane component of ABC superfamily

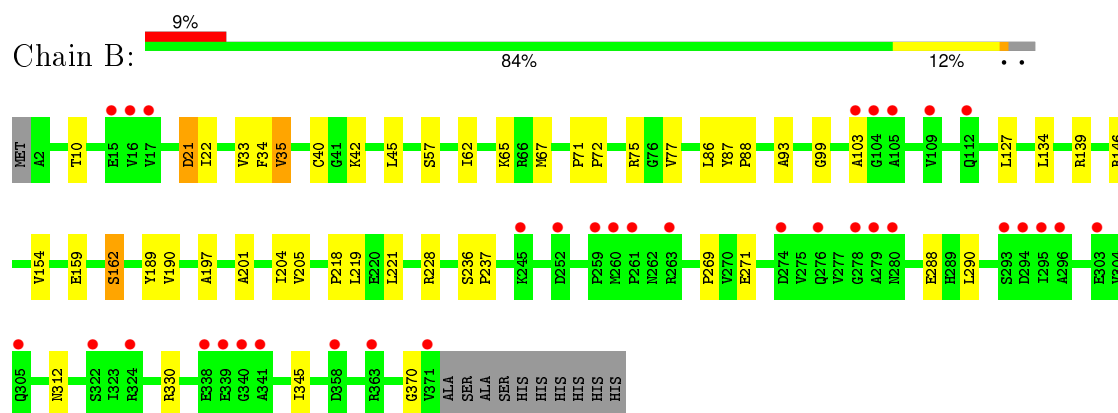


- Molecule 4: Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein





- Molecule 4: Fused maltose transport subunit, ATP-binding component of ABC superfamily; regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.02Å 93.36Å 119.76Å 90.05° 102.57° 105.01°	Depositor
Resolution (Å)	19.95 – 2.90 19.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.0 (19.95-2.90) 76.6 (19.90-2.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.237 , 0.279 0.234 , 0.275	Depositor DCC
$R_{free}$ test set	2864 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55543 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, MG, ANP, MAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	E	0.31	0/2949	0.45	0/4001
2	F	0.33	0/3823	0.47	0/5203
3	G	0.34	0/2242	0.48	0/3065
4	A	0.30	0/2921	0.48	0/3961
4	B	0.30	0/2921	0.47	0/3961
All	All	0.32	0/14856	0.47	0/20191

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2880	0	2859	29	0
2	F	3732	0	3759	28	0
3	G	2182	0	2271	20	0
4	A	2871	0	2936	36	0
4	B	2871	0	2937	30	0
5	E	23	0	22	0	0
5	F	23	0	22	2	0
6	F	51	0	76	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	27	0	12	0	0
8	B	27	0	12	0	0
9	A	3	0	0	0	0
9	B	5	0	0	0	0
All	All	14697	0	14906	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:236:SER:HB3	4:B:237:PRO:HD3	1.54	0.89
4:A:236:SER:HB3	4:A:237:PRO:HD3	1.58	0.84
3:G:91:VAL:O	3:G:95:SER:HB2	1.82	0.78
4:A:159:GLU:HB3	4:A:162:SER:HB2	1.67	0.75
1:E:277:LYS:HD3	2:F:200:SER:HB3	1.71	0.71
2:F:387:LEU:HD21	2:F:429:LEU:HD13	1.72	0.71
4:B:159:GLU:HB3	4:B:162:SER:HB2	1.78	0.66
1:E:278:GLU:HG2	2:F:200:SER:HB2	1.77	0.65
2:F:388:CYS:O	2:F:392:LEU:HB2	1.97	0.65
4:A:236:SER:CB	4:A:237:PRO:HD3	2.27	0.64
3:G:166:TYR:CE1	3:G:229:GLU:HG2	2.33	0.64
4:B:236:SER:CB	4:B:237:PRO:HD3	2.28	0.63
2:F:392:LEU:HD13	2:F:422:LEU:HD11	1.81	0.63
1:E:339:PHE:HA	1:E:368:ILE:HD12	1.81	0.63
2:F:406:ASP:HB3	4:B:99:GLY:HA2	1.81	0.63
4:B:77:VAL:HG23	4:B:154:VAL:HB	1.81	0.62
3:G:17:HIS:O	3:G:21:LEU:HB2	1.99	0.62
4:B:288:GLU:HG3	4:B:330:ARG:HD3	1.82	0.61
4:A:321:PRO:O	4:A:322:SER:HB2	2.01	0.60
1:E:68:GLY:HA3	1:E:332:ASN:O	2.02	0.60
2:F:275:LYS:HB3	2:F:276:PRO:HD3	1.84	0.60
3:G:166:TYR:CZ	3:G:229:GLU:HG2	2.37	0.59
3:G:274:ILE:H	3:G:274:ILE:HD12	1.65	0.59
1:E:48:PRO:HG3	1:E:70:TYR:HE1	1.67	0.58
4:B:33:VAL:HG22	4:B:189:TYR:HB3	1.85	0.58
4:A:33:VAL:HG22	4:A:189:TYR:HB3	1.85	0.57
3:G:166:TYR:OH	3:G:229:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:PHE:HD2	4:A:205:VAL:HB	1.69	0.57
4:A:312:ASN:HB2	4:B:288:GLU:HG2	1.86	0.57
4:A:35:VAL:HG11	4:A:197:ALA:HB2	1.87	0.57
1:E:321:MET:O	1:E:325:GLN:HG2	2.06	0.56
4:A:288:GLU:HG2	4:B:312:ASN:HB2	1.88	0.56
3:G:29:PHE:HB3	3:G:30:PRO:HD3	1.88	0.56
4:B:236:SER:HB3	4:B:237:PRO:CD	2.33	0.56
1:E:85:PHE:HA	1:E:88:LYS:HE3	1.87	0.56
4:A:26:ILE:HG12	4:A:32:VAL:HG21	1.87	0.55
1:E:122:LEU:HD21	1:E:126:PRO:HD3	1.87	0.55
2:F:437:ASN:HD21	5:F:2001:MAL:H62	1.71	0.55
4:A:77:VAL:HG23	4:A:154:VAL:HB	1.89	0.55
1:E:48:PRO:HG3	1:E:70:TYR:CE1	2.41	0.54
2:F:83:LEU:O	2:F:86:THR:HG22	2.07	0.53
1:E:97:VAL:HG21	1:E:107:PRO:HD3	1.90	0.53
3:G:7:LYS:HD3	3:G:12:ARG:HH22	1.73	0.53
4:A:290:LEU:HD22	4:A:345:ILE:HD13	1.91	0.53
1:E:229:PRO:HA	1:E:232:TRP:CE2	2.44	0.53
4:A:221:LEU:HB3	4:A:234:ILE:HD13	1.91	0.52
2:F:327:VAL:HG13	2:F:331:ILE:HD11	1.91	0.52
1:E:336:MET:O	1:E:339:PHE:HB3	2.10	0.51
2:F:27:VAL:HG21	2:F:54:LEU:HD11	1.91	0.51
4:A:292:PRO:HD2	4:A:295:ILE:HD12	1.93	0.51
2:F:122:PHE:HZ	2:F:176:ILE:HD13	1.74	0.51
1:E:115:LEU:HD22	1:E:248:PRO:HD3	1.92	0.51
4:A:42:LYS:HB3	4:A:190:VAL:HG13	1.93	0.51
4:B:67:MET:CE	4:B:75:ARG:HA	2.40	0.51
2:F:422:LEU:O	2:F:426:LEU:HB2	2.12	0.50
4:A:26:ILE:HD13	4:A:188:ILE:HD12	1.91	0.50
4:B:67:MET:HE2	4:B:75:ARG:HA	1.93	0.50
4:A:272:SER:O	4:A:275:VAL:HG22	2.11	0.50
2:F:378:TRP:HE3	2:F:379:LEU:HD12	1.76	0.50
4:A:327:LEU:HD21	4:A:345:ILE:HD11	1.94	0.50
2:F:122:PHE:HA	2:F:134:ALA:O	2.11	0.50
4:A:161:LEU:HB3	4:A:169:ARG:HG3	1.93	0.50
3:G:99:ILE:HG23	3:G:170:ILE:HG22	1.94	0.49
1:E:66:ARG:HD3	1:E:337:CYS:HB3	1.94	0.49
3:G:74:ILE:H	3:G:74:ILE:HD13	1.77	0.49
4:A:34:PHE:CD2	4:A:205:VAL:HB	2.48	0.49
2:F:85:CYS:O	2:F:89:ILE:HG12	2.12	0.49
4:B:35:VAL:HG11	4:B:197:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:428:PRO:HA	2:F:431:ILE:HG12	1.94	0.48
1:E:9:ILE:HG12	1:E:59:ILE:HB	1.96	0.48
4:B:34:PHE:HD2	4:B:205:VAL:HB	1.78	0.48
4:B:204:ILE:HD12	4:B:218:PRO:HA	1.95	0.48
1:E:364:ALA:O	1:E:368:ILE:HG12	2.14	0.47
4:B:33:VAL:HG23	4:B:201:ALA:HB2	1.96	0.47
4:A:5:GLN:HG3	4:A:61:PHE:HB2	1.97	0.47
1:E:314:ASP:HB3	1:E:317:ILE:HD12	1.97	0.47
1:E:278:GLU:HG3	2:F:201:LEU:HB2	1.97	0.47
4:A:35:VAL:CG1	4:A:197:ALA:HB2	2.45	0.47
6:F:4001:PGV:H82	3:G:19:LEU:HD23	1.97	0.46
2:F:60:ARG:HG2	2:F:66:ARG:HH22	1.79	0.46
4:A:67:MET:CE	4:A:75:ARG:HA	2.45	0.46
4:A:155:PHE:HB2	4:A:187:MET:HG2	1.98	0.46
4:A:309:GLN:HB3	4:B:219:LEU:HD13	1.97	0.46
4:A:236:SER:HB3	4:A:237:PRO:CD	2.37	0.46
1:E:59:ILE:HG21	1:E:280:LEU:HD21	1.96	0.46
4:A:336:LEU:HD21	4:B:370:GLY:HA2	1.97	0.45
3:G:79:PHE:HB3	3:G:84:TRP:CH2	2.52	0.45
2:F:30:LEU:O	2:F:34:MET:HG2	2.17	0.45
2:F:379:LEU:HB3	5:F:2001:MAL:H4	1.98	0.45
2:F:218:THR:HG22	2:F:229:ARG:HG2	1.98	0.45
3:G:86:TRP:NE1	3:G:90:LYS:HD2	2.32	0.45
4:A:138:GLN:O	4:A:142:VAL:HG23	2.17	0.45
2:F:119:THR:HG22	2:F:205:SER:HB3	1.98	0.45
1:E:66:ARG:HD3	1:E:337:CYS:CB	2.47	0.44
3:G:52:GLU:CD	3:G:52:GLU:H	2.20	0.44
2:F:381:TYR:N	2:F:382:PRO:HD2	2.32	0.44
4:B:290:LEU:HD22	4:B:345:ILE:HD13	1.99	0.44
1:E:125:PRO:HA	1:E:126:PRO:HD3	1.91	0.44
2:F:444:ILE:HG13	2:F:466:LEU:HG	2.00	0.44
4:B:86:LEU:HA	4:B:146:ARG:NH2	2.33	0.44
4:A:87:TYR:HA	4:A:88:PRO:HD3	1.87	0.44
2:F:183:LEU:HA	2:F:186:ILE:HD12	1.99	0.43
4:B:33:VAL:CG2	4:B:201:ALA:HB2	2.48	0.43
3:G:208:LEU:N	3:G:209:PRO:HD2	2.33	0.43
1:E:259:VAL:O	1:E:330:MET:HB2	2.19	0.43
1:E:333:ILE:HD12	1:E:335:GLN:HB2	2.01	0.43
1:E:126:PRO:HB3	1:E:131:GLU:HG3	2.00	0.43
4:A:42:LYS:HB3	4:A:190:VAL:CG1	2.49	0.42
4:A:236:SER:CB	4:A:237:PRO:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:40:CYS:SG	4:B:42:LYS:HG3	2.60	0.42
2:F:67:TYR:HB2	3:G:109:ALA:HB2	2.00	0.42
4:B:22:ILE:HD11	4:B:45:LEU:HD21	2.01	0.42
4:B:134:LEU:HB2	4:B:139:ARG:HG3	2.01	0.42
1:E:136:ASP:O	1:E:140:LYS:HB2	2.19	0.42
1:E:279:PHE:O	1:E:283:TYR:HB2	2.19	0.41
4:B:34:PHE:HB2	4:B:190:VAL:HG22	2.02	0.41
4:A:288:GLU:HG3	4:A:330:ARG:HD3	2.02	0.41
4:A:261:PRO:HD3	4:A:322:SER:OG	2.20	0.41
3:G:212:VAL:N	3:G:213:PRO:HD2	2.35	0.41
4:A:352:CYS:O	4:A:364:ARG:HD3	2.21	0.41
4:B:93:ALA:HB2	4:B:127:LEU:HB3	2.03	0.41
4:B:10:THR:HB	4:B:57:SER:HB3	2.02	0.41
1:E:47:PHE:HB3	1:E:48:PRO:HD3	2.02	0.41
1:E:193:THR:HA	1:E:357:VAL:HG21	2.02	0.41
4:A:62:ILE:HD12	4:A:67:MET:HG3	2.03	0.41
3:G:5:GLN:HA	3:G:6:PRO:HD3	1.97	0.41
4:B:87:TYR:HA	4:B:88:PRO:HD3	1.85	0.40
3:G:129:GLN:NE2	3:G:172:LEU:HG	2.36	0.40
3:G:7:LYS:C	3:G:9:GLN:H	2.23	0.40
2:F:332:SER:O	2:F:335:ILE:HG13	2.21	0.40
4:A:46:LEU:HG	4:A:156:LEU:HB3	2.04	0.40
1:E:314:ASP:HA	1:E:315:PRO:HD2	1.95	0.40
4:B:62:ILE:HD12	4:B:67:MET:HG3	2.04	0.40
4:B:71:PRO:HA	4:B:72:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	368/370 (100%)	354 (96%)	12 (3%)	2 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	477/514 (93%)	457 (96%)	18 (4%)	2 (0%)	39 74
3	G	280/296 (95%)	258 (92%)	17 (6%)	5 (2%)	11 37
4	A	368/381 (97%)	349 (95%)	18 (5%)	1 (0%)	46 79
4	B	368/381 (97%)	354 (96%)	11 (3%)	3 (1%)	24 60
All	All	1861/1942 (96%)	1772 (95%)	76 (4%)	13 (1%)	26 63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	173	ASN
2	F	355	PHE
3	G	8	SER
4	B	103	ALA
2	F	58	ALA
3	G	3	MET
3	G	71	ASP
4	B	21	ASP
3	G	230	VAL
4	A	21	ASP
1	E	165	GLY
3	G	7	LYS
4	B	269	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	298/298 (100%)	294 (99%)	4 (1%)	76 94
2	F	391/424 (92%)	379 (97%)	12 (3%)	47 82
3	G	228/237 (96%)	214 (94%)	14 (6%)	23 56
4	A	314/323 (97%)	307 (98%)	7 (2%)	60 88
4	B	314/323 (97%)	307 (98%)	7 (2%)	60 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1545/1605 (96%)	1501 (97%)	44 (3%)	51 84

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	45	GLU
1	E	128	THR
1	E	258	PHE
1	E	358	ASP
2	F	57	PHE
2	F	86	THR
2	F	103	GLU
2	F	176	ILE
2	F	187	THR
2	F	210	LEU
2	F	216	ASP
2	F	325	TYR
2	F	331	ILE
2	F	339	LEU
2	F	440	ASN
2	F	453	ASP
3	G	7	LYS
3	G	9	GLN
3	G	15	ILE
3	G	19	LEU
3	G	21	LEU
3	G	52	GLU
3	G	54	ILE
3	G	61	LEU
3	G	74	ILE
3	G	75	THR
3	G	83	LEU
3	G	122	LEU
3	G	146	ARG
3	G	172	LEU
4	A	65	LYS
4	A	100	LEU
4	A	270	VAL
4	A	271	GLU
4	A	324	ARG
4	A	334	VAL
4	A	350	GLU

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Mol	Chain	Res	Type
4	B	21	ASP
4	B	35	VAL
4	B	65	LYS
4	B	162	SER
4	B	221	LEU
4	B	228	ARG
4	B	271	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	181	GLN
2	F	437	ASN
2	F	440	ASN
4	B	116	GLN
4	B	255	GLN
4	B	264	GLN
4	B	289	HIS
4	B	366	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ANP	A	2501	7	22,29,33	1.51	3 (13%)	24,45,52	2.09	5 (20%)
8	ANP	B	2502	7	22,29,33	1.52	3 (13%)	24,45,52	2.09	5 (20%)
5	MAL	E	2002	-	24,24,24	0.45	0	35,35,35	0.62	0
5	MAL	F	2001	-	24,24,24	0.48	0	35,35,35	0.99	1 (2%)
6	PGV	F	4001	-	50,50,50	1.05	3 (6%)	51,56,56	1.03	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANP	A	2501	7	-	0/9/32/38	0/3/3/3
8	ANP	B	2502	7	-	0/9/32/38	0/3/3/3
5	MAL	E	2002	-	-	0/8/48/48	0/2/2/2
5	MAL	F	2001	-	-	0/8/48/48	0/2/2/2
6	PGV	F	4001	-	-	0/55/55/55	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2501	ANP	PB-O3A	2.00	1.61	1.59
8	B	2502	ANP	PB-O3A	2.12	1.61	1.59
8	B	2502	ANP	C5-C4	3.24	1.47	1.40
8	A	2501	ANP	C5-C4	3.30	1.47	1.40
6	F	4001	PGV	C12-C11	3.68	1.53	1.31
6	F	4001	PGV	O01-C1	4.01	1.46	1.34
6	F	4001	PGV	O03-C19	4.15	1.45	1.33
8	A	2501	ANP	PB-O1B	4.47	1.51	1.46
8	B	2502	ANP	PB-O1B	4.52	1.51	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2502	ANP	N3-C2-N1	-7.33	123.28	128.89
8	A	2501	ANP	N3-C2-N1	-7.32	123.29	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	A	2501	ANP	PA-O3A-PB	-3.82	122.00	132.73
8	B	2502	ANP	PA-O3A-PB	-3.09	124.06	132.73
8	B	2502	ANP	C4-C5-N7	-2.96	106.75	109.48
8	A	2501	ANP	C4-C5-N7	-2.86	106.85	109.48
8	B	2502	ANP	C2'-C1'-N9	-2.75	110.10	114.29
8	A	2501	ANP	C2'-C1'-N9	-2.17	110.98	114.29
6	F	4001	PGV	C10-C11-C12	-2.07	110.91	125.34
5	F	2001	MAL	C1'-O5'-C5'	2.03	117.23	113.47
6	F	4001	PGV	O03-C19-C20	2.69	120.10	111.90
8	A	2501	ANP	O2B-PB-O1B	2.95	117.56	110.07
8	B	2502	ANP	O2B-PB-O1B	3.01	117.71	110.07
6	F	4001	PGV	O01-C1-C2	3.89	119.98	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2001	MAL	2	0
6	F	4001	PGV	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	370/370 (100%)	-0.35	5 (1%) 78 76	44, 75, 114, 139	0
2	F	481/514 (93%)	0.04	26 (5%) 29 23	45, 89, 181, 261	0
3	G	282/296 (95%)	-0.19	10 (3%) 48 40	44, 72, 115, 143	0
4	A	370/381 (97%)	-0.03	13 (3%) 48 40	58, 88, 123, 148	0
4	B	370/381 (97%)	0.30	34 (9%) 11 7	57, 100, 215, 277	0
All	All	1873/1942 (96%)	-0.03	88 (4%) 35 29	44, 85, 166, 277	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	322	SER	7.3
2	F	18	SER	7.0
2	F	40	TYR	6.8
3	G	8	SER	6.6
4	B	276	GLN	6.1
4	B	324	ARG	5.8
2	F	19	VAL	5.7
4	B	259	PRO	5.4
4	B	261	PRO	5.4
4	B	263	ARG	5.1
2	F	29	TYR	4.8
4	B	280	ASN	4.7
2	F	41	LEU	4.5
4	B	278	GLY	4.1
4	B	279	ALA	4.1
4	A	324	ARG	4.0
2	F	35	TYR	4.0
4	B	293	SER	3.9
4	A	124	ALA	3.9
4	B	340	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
4	A	103	ALA	3.7
4	A	295	ILE	3.6
4	B	295	ILE	3.6
4	A	15	GLU	3.5
3	G	73	ARG	3.5
3	G	71	ASP	3.4
4	B	252	ASP	3.4
2	F	34	MET	3.3
4	B	105	ALA	3.3
4	B	15	GLU	3.2
1	E	174	GLY	3.2
4	B	303	GLU	3.1
3	G	7	LYS	3.1
4	B	16	VAL	3.1
4	B	338	GLU	3.1
2	F	355	PHE	3.0
4	B	260	MET	3.0
2	F	503	ILE	3.0
2	F	55	TYR	3.0
4	B	305	GLN	2.9
3	G	117	GLY	2.9
3	G	72	GLY	2.9
4	B	294	ASP	2.8
3	G	116	PRO	2.8
2	F	39	GLU	2.7
4	B	104	GLY	2.7
3	G	54	ILE	2.6
4	A	16	VAL	2.6
3	G	74	ILE	2.5
2	F	195	LYS	2.5
4	B	371	VAL	2.5
1	E	175	LYS	2.5
2	F	61	LYS	2.5
4	B	103	ALA	2.5
2	F	269	THR	2.5
4	B	339	GLU	2.4
1	E	173	ASN	2.4
2	F	194	ASN	2.4
2	F	463	TYR	2.4
4	A	261	PRO	2.4
1	E	172	GLU	2.4
4	A	128	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	109	VAL	2.4
4	B	341	ALA	2.4
2	F	217	GLY	2.4
4	A	13	TRP	2.4
4	B	274	ASP	2.3
2	F	241	THR	2.3
4	B	245	LYS	2.3
4	B	296	ALA	2.3
4	B	17	VAL	2.3
4	A	95	ASN	2.2
4	A	49	ILE	2.2
2	F	23	LEU	2.2
2	F	59	ASN	2.2
2	F	353	ALA	2.2
1	E	170	LYS	2.1
2	F	253	PRO	2.1
2	F	22	LEU	2.1
3	G	183	THR	2.1
2	F	44	ILE	2.1
4	B	363	ARG	2.1
2	F	37	GLN	2.1
4	A	5	GLN	2.0
4	B	112	GLN	2.0
4	A	129	ARG	2.0
4	B	358	ASP	2.0
2	F	357	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PGV	F	4001	51/51	0.81	0.29	2.17	89,97,103,104	0
8	ANP	A	2501	27/31	0.90	0.21	0.50	72,85,94,97	0
8	ANP	B	2502	27/31	0.92	0.18	0.02	74,87,95,98	0
5	MAL	F	2001	23/23	0.94	0.14	-0.18	45,47,50,51	0
5	MAL	E	2002	23/23	0.98	0.12	-0.58	47,53,58,58	0
7	MG	A	1501	1/1	0.98	0.15	-	51,51,51,51	0
7	MG	B	1502	1/1	0.98	0.14	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.